Supporting Information for
A Computational Study of Nicotine Conformations in the Gas Phase and in Water
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Structure: ***cis*0 A**
Total Energy (HF/6-31G**): -495.7344284 au
Cartesian coordinates:

1 H	-3.5173	-1.4487	0.2240
2 C	-2.4720	-1.3410	-0.0395
3 C	-2.2609	-0.1279	-0.9600
4 N	-1.7219	0.8894	-0.0823
5 C	-0.8354	0.2436	0.8792
6 C	-1.6230	-1.0360	1.2182
7 H	-2.1719	-2.2640	-0.5241
8 H	-3.1846	0.2219	-1.4101
9 H	-1.5800	-0.3716	-1.7808
10 C	-1.2581	2.0912	-0.7271
11 H	-0.9276	2.8069	0.0182
12 H	-0.7649	0.8852	1.7520
13 C	0.5945	-0.0036	0.4022
14 H	-2.2723	-0.8323	2.0609
15 H	-0.9747	-1.8565	1.5008
16 C	3.2066	-0.2453	-0.3580
17 C	0.9689	-1.0433	-0.4419
18 C	1.6123	0.8505	0.8109
19 N	2.8784	0.7439	0.4503
20 C	2.2894	-1.1674	-0.8313
21 H	0.2457	-1.7593	-0.7879
22 H	1.3845	1.6674	1.4761
23 H	4.2439	-0.3118	-0.6386
24 H	2.6043	-1.9626	-1.4822
25 H	-2.0790	2.5420	-1.2753
26 H	-0.4355	1.9255	-1.4260

Structure: ***cis*0 B**
Total Energy (HF/6-31G**): -495.7341542 au
Cartesian coordinates:

1 H	-3.5083	-1.4483	0.2061
2 C	-2.4617	-1.3404	-0.0522
3 C	-2.2457	-0.1227	-0.9647
4 N	-1.7225	0.8934	-0.0748
5 C	-0.8382	0.2465	0.8876
6 C	-1.6189	-1.0418	1.2112
7 H	-2.1587	-2.2604	-0.5399
8 H	-3.1656	0.2251	-1.4240
9 H	-1.5529	-0.3594	-1.7769
10 C	-1.2629	2.1026	-0.7079
11 H	-0.9481	2.8178	0.0453
12 H	-0.7790	0.8813	1.7665
13 C	0.5997	0.0190	0.4205
14 H	-2.2722	-0.8494	2.0535
15 H	-0.9669	-1.8609	1.4884
16 C	3.1535	-0.3928	-0.4574
17 C	1.6113	0.8818	0.8179
18 C	0.9803	-1.0285	-0.4151
19 N	2.2111	-1.2328	-0.8454
20 C	2.9074	0.6805	0.3778
21 H	1.3879	1.7065	1.4736
22 H	0.2540	-1.7483	-0.7483
23 H	4.1473	-0.5862	-0.8236
24 H	3.7060	1.3351	0.6756
25 H	-2.0820	2.5490	-1.2625
26 H	-0.4313	1.9490	-1.3987

Structure: ***trans*0 A**
Total Energy (HF/6-31G**): -495.741669 au
Cartesian coordinates:

1 H	3.5808	-1.7776	-0.1463
2 C	2.8309	-1.2086	0.3910
3 C	2.9329	0.2891	0.0911
4 N	1.5627	0.7594	0.1724
5 C	0.7597	-0.2508	-0.5007
6 C	1.3897	-1.5786	-0.0246
7 H	2.9786	-1.3934	1.4486
8 H	3.3476	0.4496	-0.9102
9 H	3.5627	0.8243	0.7937
10 H	2.0013	2.7874	0.2601
11 C	1.3820	2.1073	-0.3145
12 H	0.8893	-0.1737	-1.5860
13 C	-0.7187	-0.1320	-0.2004
14 H	1.3559	-2.3257	-0.8094
15 H	0.8363	-1.9744	0.8181
16 C	-3.4025	-0.0174	0.2265
17 C	-1.1893	0.1140	1.0843
18 C	-1.6679	-0.2974	-1.1965
19 N	-2.9750	-0.2472	-0.9985
20 C	-2.5508	0.1739	1.3039
21 H	-0.4907	0.2660	1.8873
22 H	-1.3538	-0.4788	-2.2114
23 H	-4.4701	0.0211	0.3620
24 H	-2.9497	0.3654	2.2834
25 H	0.3505	2.4150	-0.1968
26 H	1.6516	2.2121	-1.3702

Structure: ***trans*0 B**
Total Energy (HF/6-31G**): -495.7408306 au
Cartesian coordinates:

1 C	-2.8263	-1.2077	-0.3981
2 C	-2.9299	0.2880	-0.0886
3 N	-1.5595	0.7585	-0.1584
4 C	-0.7606	-0.2560	0.5115
5 C	-1.3865	-1.5802	0.0202
6 C	-1.3800	2.1039	0.3344
7 C	0.7222	-0.1368	0.2288
8 C	3.3638	0.0190	-0.4075
9 C	1.6694	-0.3193	1.2208
10 C	1.1962	0.1272	-1.0545
11 N	2.4739	0.2046	-1.3689
12 C	3.0159	-0.2448	0.9025
13 H	-3.5780	-1.7805	0.1327
14 H	-2.9697	-1.3854	-1.4574
15 H	-3.3506	0.4419	0.9115
16 H	-3.5552	0.8281	-0.7913
17 H	-0.8992	-0.1876	1.5970
18 H	-1.3553	-2.3350	0.7978
19 H	-0.8290	-1.9663	-0.8242
20 H	-1.9981	2.7861	-0.2388
21 H	-0.3486	2.4128	0.2193
22 H	-1.6522	2.2043	1.3902
23 H	4.3989	0.0869	-0.6956
24 H	1.3621	-0.5163	2.2342
25 H	0.4944	0.2918	-1.8528
26 H	3.7745	-0.3829	1.6513

Structure: *cis*+ **A**
Total Energy (HF/6-31G**): -496.1259506 au
Cartesian coordinates:

1 H	-3.5191	-1.4379	0.1258
2 C	-2.4673	-1.3425	-0.1099
3 C	-2.2184	-0.1223	-1.0036
4 N	-1.6877	0.9207	-0.0681
5 C	-0.7968	0.1658	0.9294
6 C	-1.6368	-1.0995	1.1754
7 H	-2.1757	-2.2489	-0.6230
8 H	-3.1000	0.2619	-1.4965
9 H	-1.4534	-0.2963	-1.7460
10 C	-1.1102	2.1163	-0.7385
11 H	-2.4717	1.2464	0.4753
12 H	-0.7542	0.7934	1.8089
13 C	0.6081	-0.0374	0.4148
14 H	-2.2953	-0.9339	2.0195
15 H	-1.0030	-1.9360	1.4301
16 C	3.2073	-0.2340	-0.3580
17 C	0.9917	-1.0929	-0.4098
18 C	1.6042	0.8460	0.8141
19 N	2.8630	0.7594	0.4378
20 C	2.3083	-1.1919	-0.8073
21 H	0.2874	-1.8399	-0.7299
22 H	1.3718	1.6603	1.4815
23 H	4.2423	-0.2795	-0.6461
24 H	2.6390	-1.9937	-1.4401
25 H	-1.8829	2.5763	-1.3373
26 H	-0.2870	1.8111	-1.3629
27 H	-0.7657	2.8116	0.0125

Structure: *cis*+ **B**
Total Energy (HF/6-31G**): -496.125946 au
Cartesian coordinates:

1 H	-3.5055	-1.4428	0.1356
2 C	-2.4541	-1.3447	-0.1011
3 C	-2.2103	-0.1274	-0.9994
4 N	-1.6900	0.9239	-0.0656
5 C	-0.7963	0.1811	0.9379
6 C	-1.6242	-1.0937	1.1831
7 H	-2.1583	-2.2516	-0.6105
8 H	-3.0928	0.2496	-1.4962
9 H	-1.4417	-0.2998	-1.7383
10 C	-1.1201	2.1202	-0.7397
11 H	-0.7872	2.8236	0.0092
12 H	-0.7661	0.8099	1.8171
13 C	0.6152	-0.0059	0.4318
14 H	-2.2831	-0.9343	2.0280
15 H	-0.9821	-1.9242	1.4360
16 C	3.1525	-0.3960	-0.4648
17 C	1.6230	0.8639	0.8405
18 C	0.9861	-1.0520	-0.4057
19 N	2.2117	-1.2375	-0.8498
20 C	2.9114	0.6713	0.3880
21 H	1.4074	1.6751	1.5153
22 H	0.2677	-1.7852	-0.7292
23 H	4.1420	-0.5810	-0.8426
24 H	3.7114	1.3203	0.6899
25 H	-1.8930	2.5698	-1.3462
26 H	-0.2906	1.8185	-1.3575
27 H	-2.4789	1.2450	0.4735

Structure: ***trans*+ A**
Total Energy (HF/6-31G**): -496.1309487 au
Cartesian coordinates:

1 C	0.7511	-0.1509	0.2265
2 C	1.6078	0.5402	1.0721
3 N	2.9139	0.6015	0.9059
4 C	3.4407	-0.0309	-0.1227
5 C	2.6865	-0.7583	-1.0360
6 C	1.3225	-0.8214	-0.8539
7 H	1.2189	1.0638	1.9302
8 H	4.5084	0.0374	-0.2308
9 H	3.1630	-1.2630	-1.8550
10 H	0.7243	-1.3941	-1.5425
11 C	-0.7273	-0.1604	0.5117
12 N	-1.5232	0.6553	-0.5010
13 C	-2.9678	0.2890	-0.2749
14 C	-2.9499	-1.1240	0.3394
15 C	-1.4642	-1.4976	0.4718
16 H	-0.9164	0.3287	1.4600
17 C	-1.2629	2.1195	-0.4882
18 H	-0.2222	2.2957	-0.7102
19 H	-1.5044	2.5053	0.4913
20 H	-1.8871	2.5908	-1.2334
21 H	-3.3789	1.0248	0.4007
22 H	-3.4891	0.3601	-1.2185
23 H	-3.4338	-1.1053	1.3069
24 H	-3.4879	-1.8302	-0.2778
25 H	-1.2528	-2.0751	1.3612
26 H	-1.1363	-2.0849	-0.3782
27 H	-1.2584	0.3166	-1.4123

Structure: ***trans*+ B**
Total Energy (HF/6-31G**): -496.1309106 au
Cartesian coordinates:

1 H	-3.4583	-1.2015	1.2277
2 C	-2.9379	-1.1516	0.2806
3 C	-2.9643	0.2953	-0.2479
4 N	-1.5230	0.6764	-0.4624
5 C	-0.7277	-0.1619	0.5298
6 C	-1.4490	-1.5070	0.4422
7 H	-3.4372	-1.8288	-0.3985
8 H	-3.3684	0.9883	0.4758
9 H	-3.4950	0.4230	-1.1802
10 H	-1.8938	2.6293	-1.1431
11 C	-1.2703	2.1406	-0.4087
12 H	-0.9284	0.2957	1.4914
13 C	0.7537	-0.1329	0.2542
14 H	-1.2515	-2.1005	1.3243
15 H	-1.0904	-2.0716	-0.4102
16 C	3.4099	-0.1329	-0.3089
17 C	1.6355	0.4486	1.1582
18 C	1.2980	-0.6933	-0.8963
19 N	2.5827	-0.6861	-1.1777
20 C	2.9872	0.4457	0.8780
21 H	1.2743	0.8893	2.0717
22 H	0.6717	-1.1757	-1.6304
23 H	4.4535	-0.1515	-0.5664
24 H	3.6974	0.8788	1.5565
25 H	-0.2296	2.3271	-0.6228
26 H	-1.5174	2.4983	0.5800
27 H	-1.2557	0.3642	-1.3825

Structure: *cis*++ **A**
Total Energy (HF/6-31G**): -496.3924632 au
Cartesian coordinates:

1 H	3.4454	-1.2765	-0.8724
2 C	2.9743	-1.1219	0.0927
3 C	2.8824	0.3570	0.4216
4 N	1.7027	0.8356	-0.4072
5 C	0.7766	-0.3873	-0.6267
6 C	1.5076	-1.5487	0.0744
7 H	3.5544	-1.6573	0.8317
8 H	3.7480	0.9488	0.1618
9 H	2.6332	0.5269	1.4605
10 H	1.9088	2.8551	0.1078
11 H	0.7359	1.9812	1.0881
12 H	0.8080	-0.5504	-1.6948
13 C	-0.6797	-0.1958	-0.2347
14 H	1.3346	-2.4751	-0.4565
15 H	1.1480	-1.6813	1.0880
16 H	0.3361	2.4444	-0.5770
17 H	2.0769	1.0472	-1.3180
18 C	1.1194	2.1180	0.0897
19 C	-3.3854	-0.0240	0.3463
20 C	-1.1365	-0.1748	1.0915
21 C	-1.6355	-0.1375	-1.2213
22 N	-2.9345	-0.0562	-0.9072
23 C	-2.4847	-0.0784	1.3860
24 H	-0.4405	-0.2418	1.9080
25 H	-1.4093	-0.1674	-2.2704
26 H	-3.6032	-0.0284	-1.6552
27 H	-2.8368	-0.0606	2.3994
28 H	-4.4484	0.0386	0.4829

Structure: ***cis*++ B**
Total Energy (HF/6-31G**): -496.3920816 au
Cartesian coordinates:

1	H	-3.2044	1.0713	-1.5365
2	C	-2.9924	1.0142	-0.4759
3	C	-3.0679	-0.4319	0.0194
4	N	-1.6193	-0.9540	0.0157
5	C	-0.7736	0.1721	-0.5878
6	C	-1.5488	1.4288	-0.1969
7	H	-3.7129	1.6352	0.0377
8	H	-3.6626	-1.0833	-0.6027
9	H	-3.4218	-0.5003	1.0361
10	H	-1.9240	-2.1992	1.6765
11	H	-1.2157	-0.6317	2.0660
12	H	-0.8872	0.0412	-1.6570
13	C	0.7154	0.0966	-0.2861
14	H	-1.2330	2.2809	-0.7843
15	H	-1.4202	1.6717	0.8534
16	H	-0.2283	-1.8970	1.3080
17	H	-1.5798	-1.7459	-0.6044 0
18	C	-1.2092	-1.4525	1.3646
19	C	3.4562	0.0555	0.1268
20	C	1.3229	0.9141	0.6373
21	C	1.5503	-0.7510	-1.0289
22	C	2.9178	-0.7850	-0.8201
23	N	2.6494	0.8665	0.8119
24	H	0.8017	1.6278	1.2440
25	H	1.1306	-1.3846	-1.7915
26	H	3.5570	-1.4331	-1.3880
27	H	3.0605	1.4856	1.4864
28	H	4.5054	0.1082	0.3484

Structure: ***trans*++ A**
Total Energy (HF/6-31G**): -496.3975303 au
Cartesian coordinates:

1 H	3.4441	-1.3412	-1.2538
2 C	2.9394	-1.2255	-0.3048
3 C	3.0445	0.2359	0.1644
4 N	1.6208	0.6661	0.4749
5 C	0.7688	-0.1373	-0.4803
6 C	1.4313	-1.5188	-0.4314
7 H	3.4107	-1.9001	0.3958
8 H	3.4035	0.8958	-0.6121
9 H	3.6415	0.3852	1.0518
10 H	2.1315	2.5964	1.1344
11 C	1.4309	2.1466	0.4464
12 H	0.9471	0.3137	-1.4489
13 C	-0.7204	-0.0926	-0.1830
14 H	1.1871	-2.0925	-1.3149
15 H	1.0746	-2.0802	0.4254
16 H	0.4223	2.3870	0.7468
17 H	1.6235	2.5025	-0.5550
18 H	1.4224	0.3563	1.4140
19 C	-3.4655	-0.0882	0.1944
20 C	-1.2925	-0.6387	0.9748
21 C	-1.5826	0.4335	-1.1157
22 N	-2.9041	0.4171	-0.9034
23 C	-2.6617	-0.6293	1.1726
24 H	-0.6740	-1.0873	1.7324
25 H	-1.2618	0.8633	-2.0457
26 H	-3.5034	0.7998	-1.6120
27 H	-3.1031	-1.0448	2.0578
28 H	-4.5365	-0.0500	0.2587

Structure: ***trans*++ B**
Total Energy (HF/6-31G**): -496.3959968 au
Cartesian coordinates:

1 H	-3.3735	-1.0756	1.4435
2 C	-2.9582	-1.1498	0.4476
3 C	-3.0455	0.2162	-0.2573
4 N	-1.6059	0.6277	-0.5426
5 C	-0.7737	-0.1233	0.4756
6 C	-1.4610	-1.4899	0.5050
7 H	-3.5191	-1.9061	-0.0824
8 H	-3.4737	0.9825	0.3713
9 H	-3.5753	0.2028	-1.1981
10 H	-2.1039	2.5168	-1.3198
11 C	-1.4181	2.1082	-0.5924
12 H	-0.9629	0.3849	1.4130
13 C	0.7250	-0.0852	0.2136
14 H	-1.1888	-2.0443	1.3928
15 H	-1.1746	-2.0865	-0.3552
16 H	-0.4040	2.3348	-0.8852
17 H	-1.6334	2.5195	0.3828
18 H	-1.3753	0.2693	-1.4562
19 C	3.4741	-0.0764	-0.1506
20 C	1.5546	0.7671	0.9564
21 C	1.3423	-0.9210	-0.6887
22 N	2.6706	-0.8857	-0.8436
23 C	2.9275	0.7792	0.7763
24 H	1.1247	1.4217	1.6942
25 H	0.8276	-1.6387	-1.2974
26 H	3.0875	-1.5141	-1.5058
27 H	3.5625	1.4288	1.3473
28 H	4.5262	-0.1421	-0.3537